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ComPASS

Advanced Computation for HEP Accelerator Science and Technology

Panagiotis Spentzouris (Fermilab)
for the ComPASS collaboration

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Accelerators for America's Future

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Particle accelerators enable discovery in basic research and applied sciences

- Probing fundamental laws of nature, discovering new particles
- Studying properties of nuclear matter
- Studying structure of crystals, amorphous materials, and organic matter
- Enhancing quality of life: medical treatment, nuclear waste transmutation, industrial applications

Numerical modeling and simulation are essential for the development of new acceleration concepts and technologies and for machine design, optimization and successful operation

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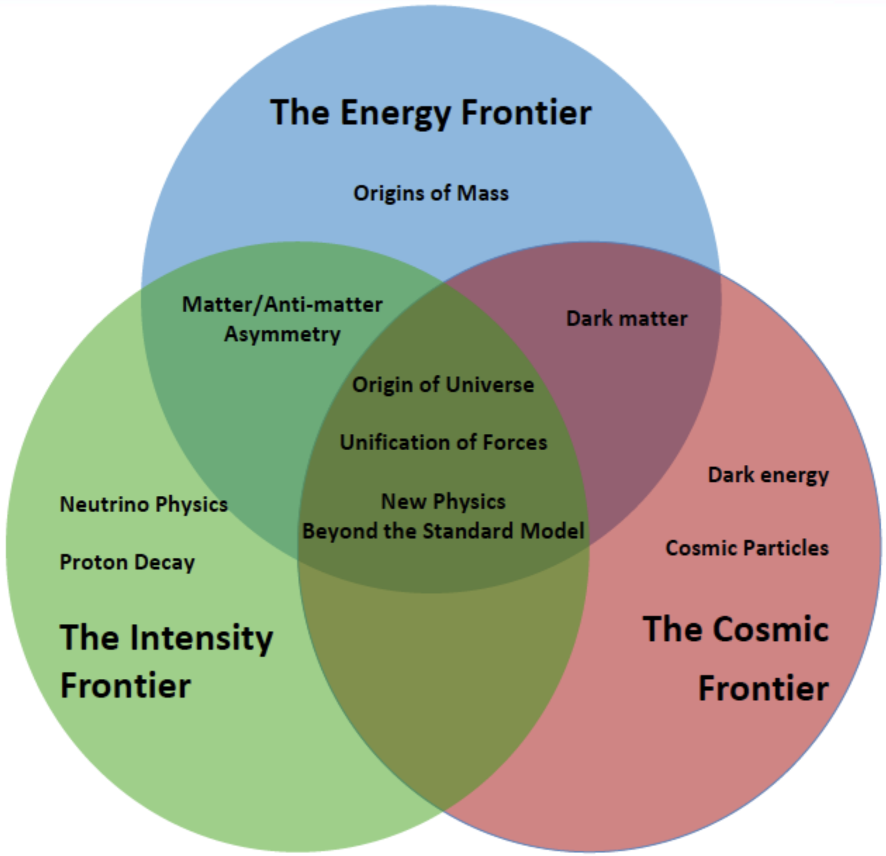
Accelerators for High Energy Physics

- At the Energy Frontier, high-energy particle beam collisions seek to uncover new phenomena
  - the origin of mass, the nature of dark matter, extra dimensions of space.
- At the Intensity Frontier, high-flux beams enable exploration of
  - neutrino interactions, to answer questions about the origins of the universe, matter-antimatter asymmetry, force unification.
  - rare processes, to open a doorway to realms to ultra-high energies, close to the unification scale
- Particle accelerators indirectly support the cosmic frontier by providing measurements of relevant physics processes



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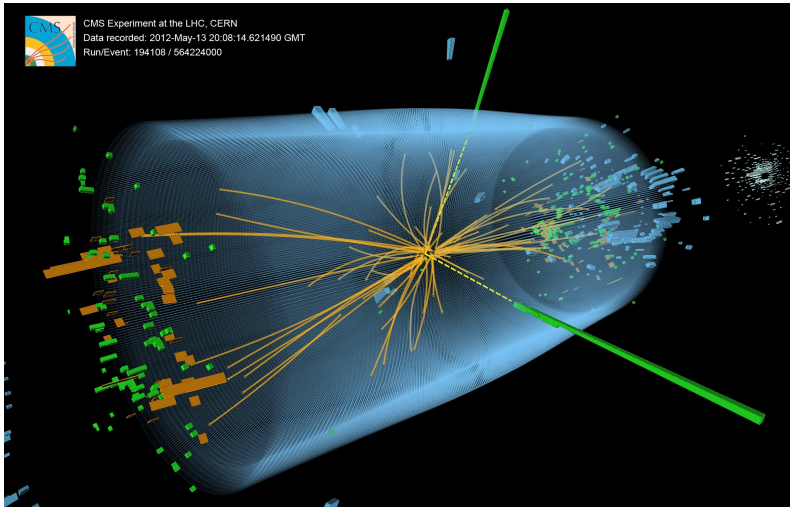
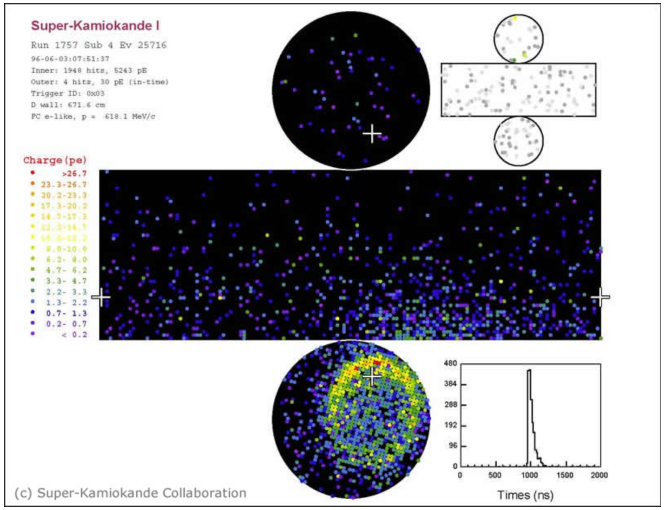
Where we are today

- Discovery of the Higgs particle, responsible for electroweak symmetry breaking and the mass of elementary particles
  - No physics beyond the “Standard Model” (SM) of HEP has been observed
- Neutrinos oscillate, thus have mass
  - No answers on mass hierarchy or symmetry properties





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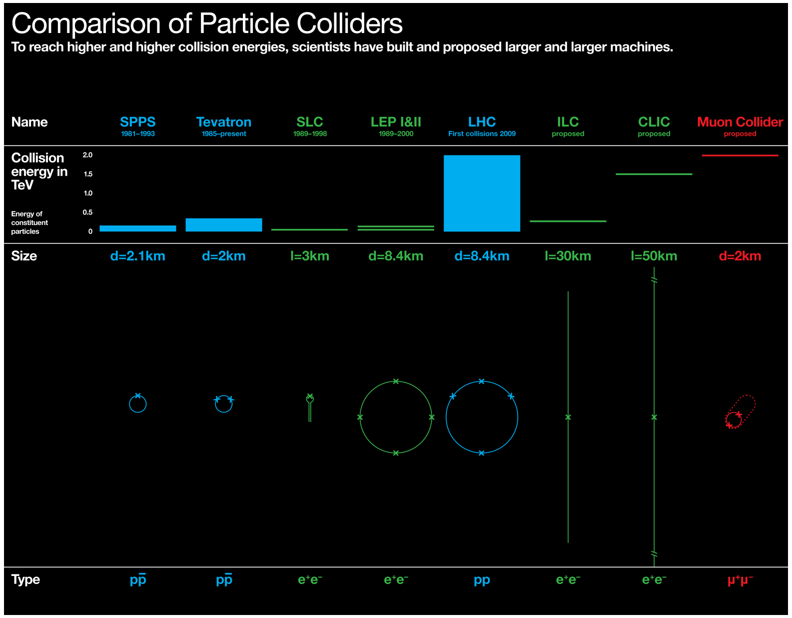
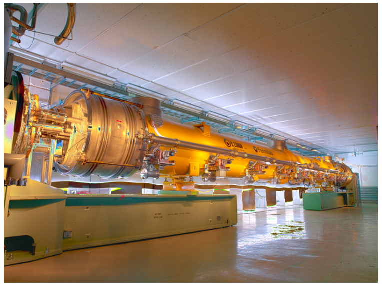
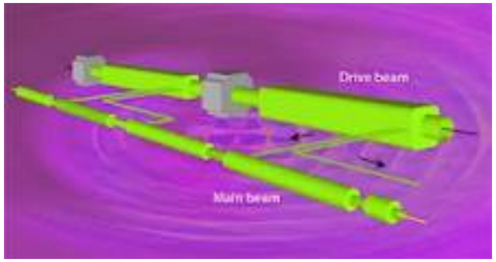
Where we would like to be (Energy Frontier)

- A dedicated accelerator will be necessary to study Higgs properties
  - Is it a "Standard Model" Higgs?
- "Higgs Factory" candidate: lepton collider
- A great challenge for accelerator science!
  - Develop techniques, technologies and materials to achieve higher acceleration gradients
    - dielectric and plasma wave structures, beam cooling
  - Optimize existing technologies
    - Superconducting rf cavities
  - Optimize and test designs
    - CLIC, Muon Collider

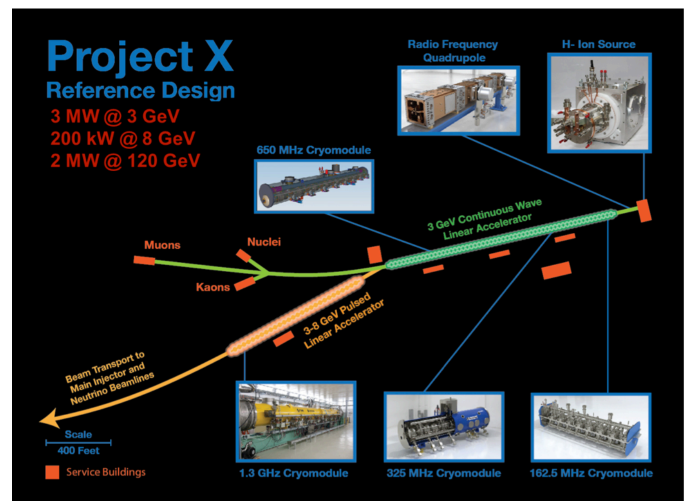






Where we would like to be (Intensity Frontier)

- A high-intensity proton accelerator to drive
  - long-baseline neutrino oscillation experiments
    - Mass hierarchy, matter-antimatter asymmetry, oscillation parameters
  - muon, kaon experiments
    - Physics beyond the SM
- Staged approach at Fermilab
  - Improvements of existing machines
  - New linear accelerator: Project-X
- A great challenge for accelerator science!
  - Controlling instabilities to minimize beam losses is essential
    - Self-fields, wakefields, interaction with materials, geometry and long term tracking accuracy



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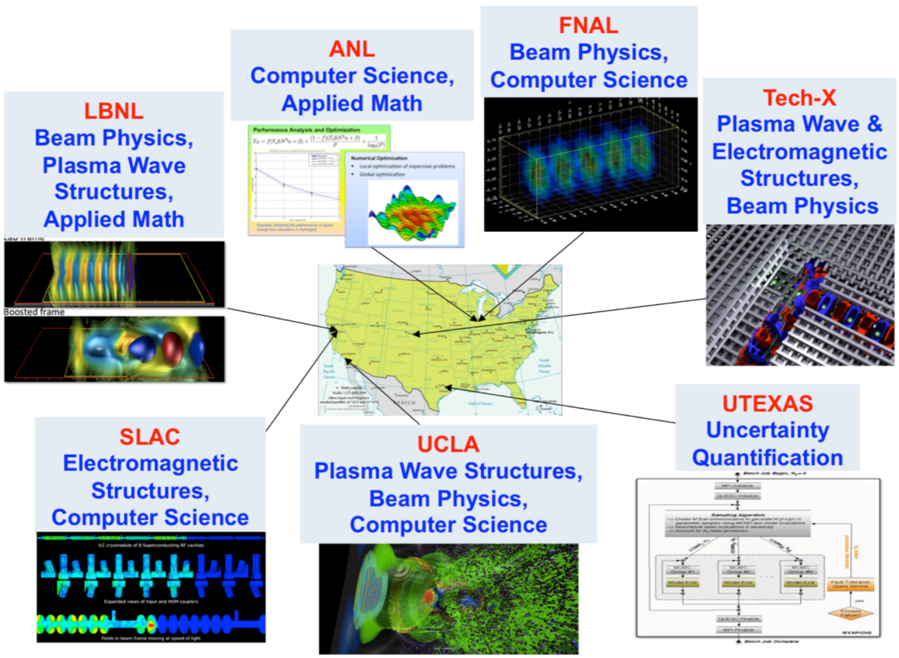
Advanced Computation for HEP Accelerator Science and Technology

- To enable scientific discovery in HEP, high-fidelity simulations are necessary to develop new designs, concepts and technologies for particle accelerators
- Under SciDAC3, ComPASS will develop and deploy state-of-the-art accelerator modeling tools that utilize
  - the most advanced algorithms on the latest most powerful supercomputers
  - cutting-edge non-linear parameter optimization and uncertainty quantification methods.

The ComPASS collaboration



Community Project for Accelerator Science and Simulation (ComPASS)

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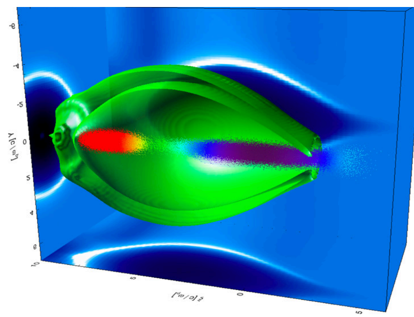
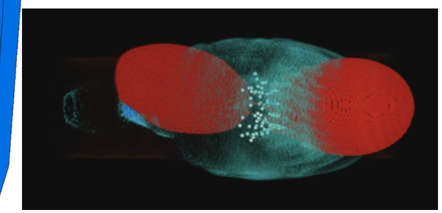
ComPASS SciDAC3 applications

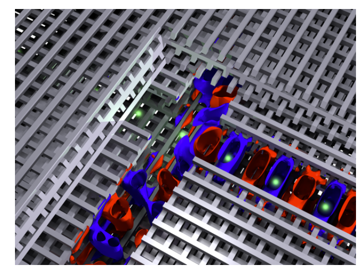
- Support the development and study of new technologies for smaller and possibly cheaper energy frontier accelerators:
  - accelerators based on standard technology are limited by the metallic electrical breakdown limit of 50-100 MV/m
  - dielectric laser accelerators: a laser propagating through a dielectric lattice can generate electric fields of few GV/m
  - plasma based acceleration: a driver beam (laser/particles) propagating through a plasma creates a wake with accelerating gradients exceeding 50 GV/m.
- Focus on plasma and dielectric R&D and optimization of conventional technology applications
- Support the design and optimization of high-intensity proton accelerators to minimize beam losses that cause radiation damage. Modeling of
  - many (all) beam bunches in circular machines and their coupling through impedance and wakefields
  - beam self-charge and instabilities caused by beam-matter interactions
  - field non-linearities and accelerator geometry
- Focus on Fermilab existing proton source improvements and Project-X

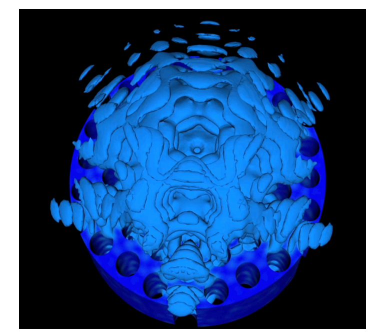
Energy Frontier Applications

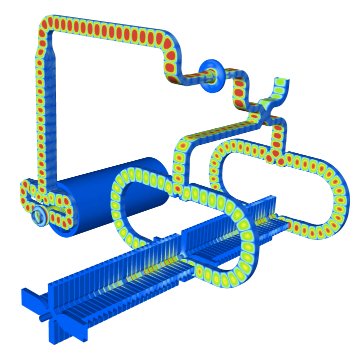
- **Plasma-based acceleration:**
  - support the BELLA (laser) and FACET (beam) experimental programs
  - develop techniques to improve beam quality
  - study controlled electron beam injection
  - improve staging for future lepton collider concepts.
- **Dielectric laser acceleration:**
  - design efficient power couplers between optical fiber and accelerator structure
  - explore wakefield effects and associated break-ups for different topologies
  - design structures able to accelerate high quality beams
- **High Gradient acceleration:**
  - understand wakefields in the Power Extraction and Transfer Structure (PETS) system of CLIC











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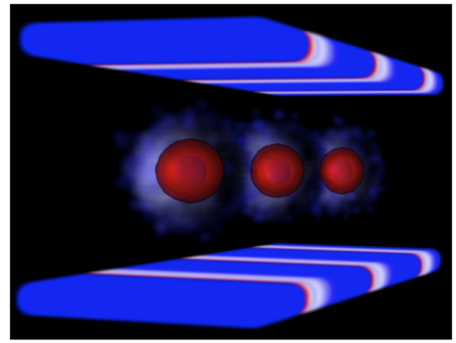
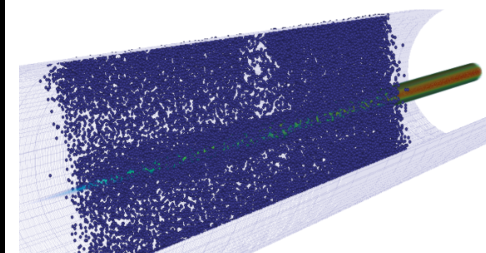
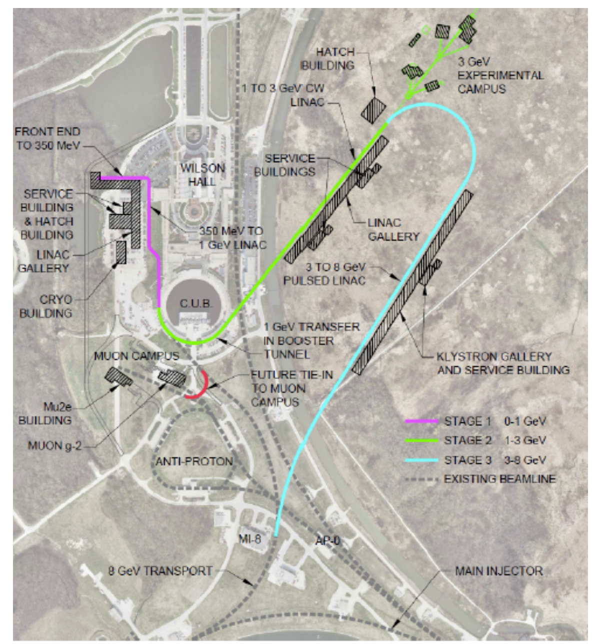
Intensity Frontier Applications

- Fermilab proton source upgrades for the Neutrino and Muon Programs
  - Booster synchrotron: instability control for beam quality and loss minimization (targeting 50% increase of beam flux)
  - Main Injector (MI) synchrotron: instability mitigation and loss minimization (targeting 100% increase of beam flux)
- Project-X: support staging
  - Study wakefields for the first stage of the linac
  - Model experiments of electron-cloud effects in the MI, currently underway
  - Study mitigation techniques to control losses in MI due to self-fields, wakefields, and electron-clouds







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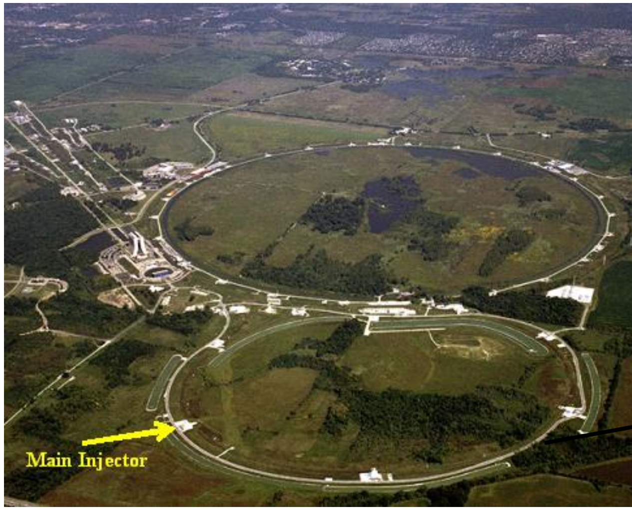
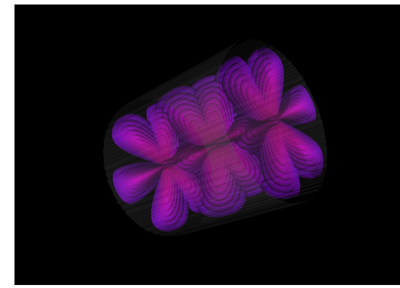
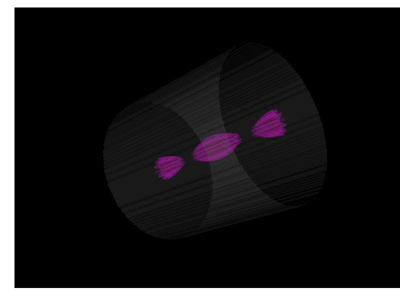
Accelerator applications span a wide range of physics and scales







- Wide range of scales:
  - accelerator complex (10^3m) → EM wavelength (10^2-10 m) → component (10-1 m) → particle bunch (10^{-3} m) → beam in plasma wakefields (10^{-8})
- Advancing accelerator science requires development of a wide range of mathematical models and numerical algorithms!

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ComPASS Methods and Tools

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- We are developing a comprehensive set of codes that incorporate state-of-the-art field solvers
  - Electrostatic: multigrid (*Synergia*, *Warp*-FastMATH); AMR multigrid (*Warp*-FastMATH)
  - Electrostatic: spectral (*Synergia*)
  - Electromagnetic: finite element direct and hybrid (*ACE3P*-FastMATH)
  - Electromagnetic: extended stencil finite-difference (*Osiris*, *Vorpal*, *Warp*-FastTMATH); AMR finite-difference (*Warp*-FastMATH)
  - Quasi-static: spectral (*QuickPIC*)

- Collaboration with SciDAC Institutes
  - FastMATH: Particle in Cell techniques, field solvers (Chombo); linear algebra solvers (SuperLU) and eigensolvers
  - QUEST: statistical calibrations and quantitative ranking of models for plasma applications (QUESO)
  - SDAV: visualization (ParaView, VisIt), indexing (FastBit); domain customized applications*
  - SUPER: performance analysis & optimization, non-linear parameter optimization.

ComPASS toolkit: ACE3P, Osiris, QuickPIC, Synergia, Vorpal, Warp

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ComPASS collaboration building on tools, expertise and partnerships developed under SciDAC2

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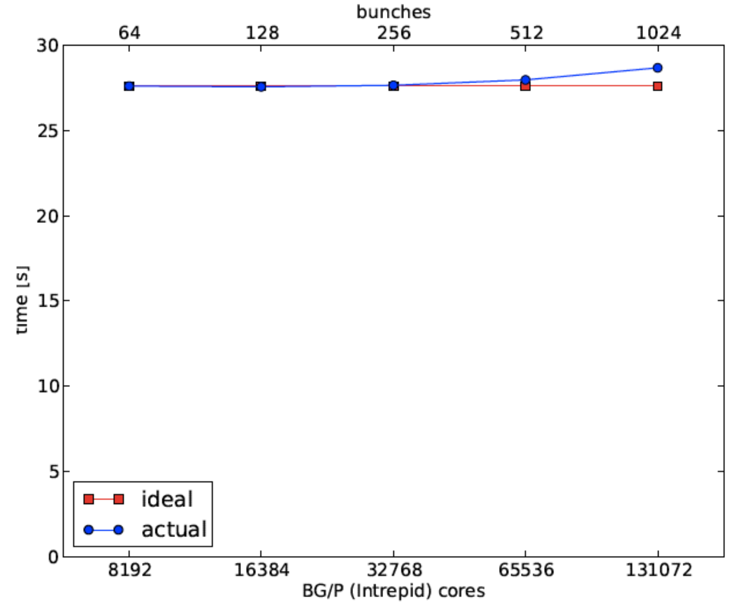
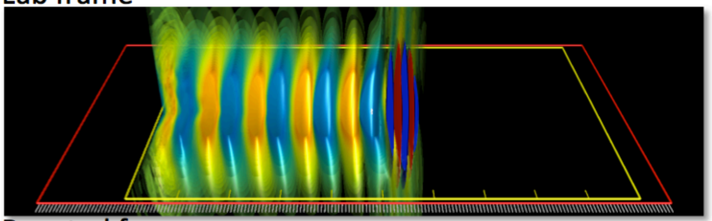
- Enabled by our partnerships with computer scientists and applied mathematicians, ComPASS codes have
  - improved parallelism both at the MPI and node level, better data partitioning
    - allowing realistic multi-physics, multi-scale simulations
  - new techniques and algorithms
    - allowing modeling of previously computationally prohibitive problems
  - prototypes of algorithms and computational framework infrastructure on modern architectures (CUDA-GPU)

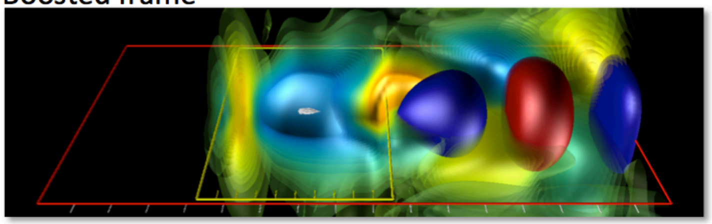


Synergia MI full machine simulations

Lab frame



Boosted frame



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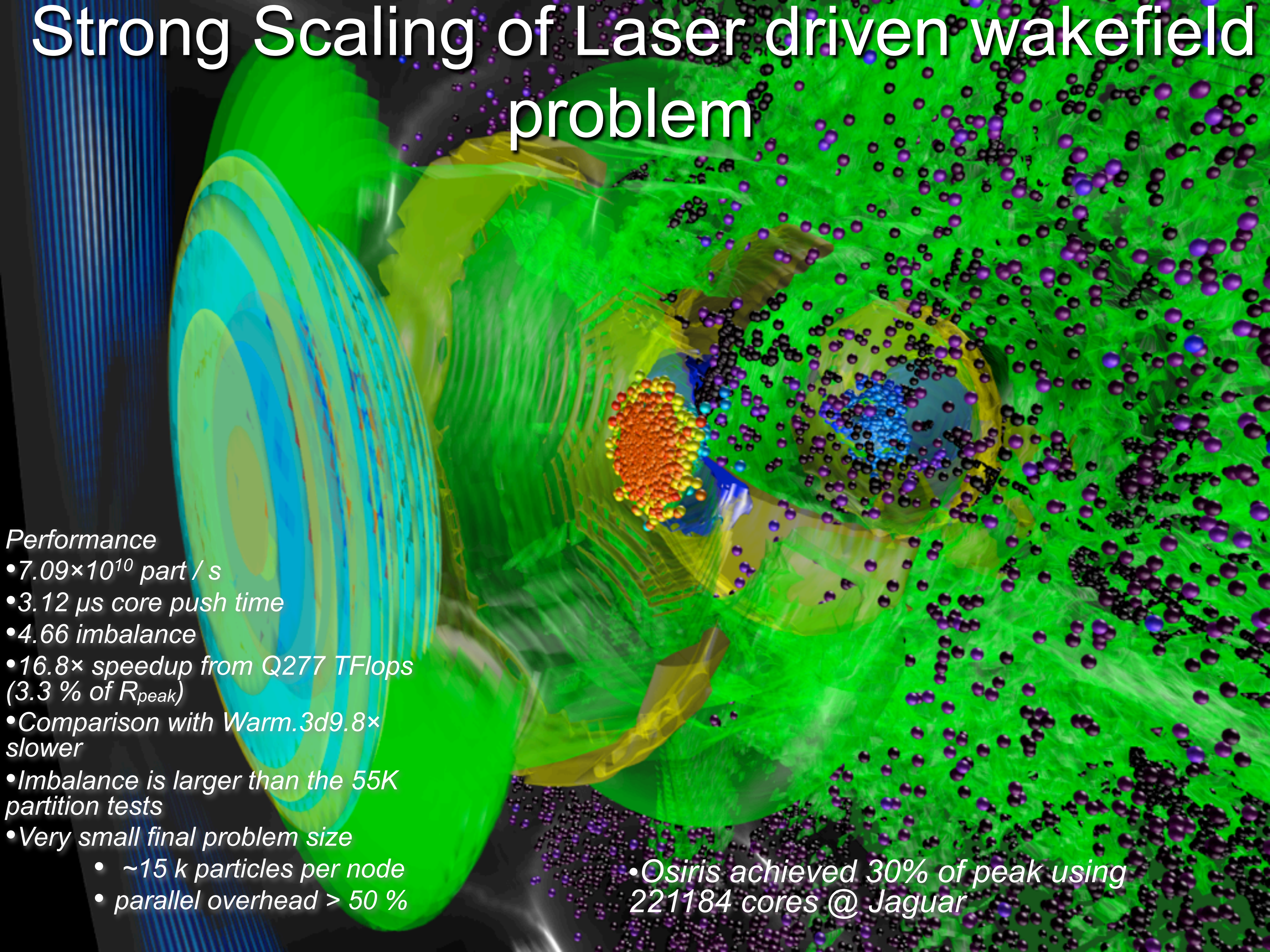
Strong Scaling of Laser driven wakefield problem



Performance

- *7.09×10^{10} part / s*
- *3.12 μs core push time*
- *4.66 imbalance*
- *16.8× speedup from Q277 TFlops (3.3 % of R_{peak})*
- *Comparison with Warm.3d9.8× slower*
- *Imbalance is larger than the 55K partition tests*
- *Very small final problem size*
  - *~15 k particles per node*
  - *parallel overhead > 50 %*

- *Osiris achieved 30% of peak using 221184 cores @ Jaguar*

Plasma-based acceleration is rich in science:

➢ Compass codes have been essential to the progress of this field

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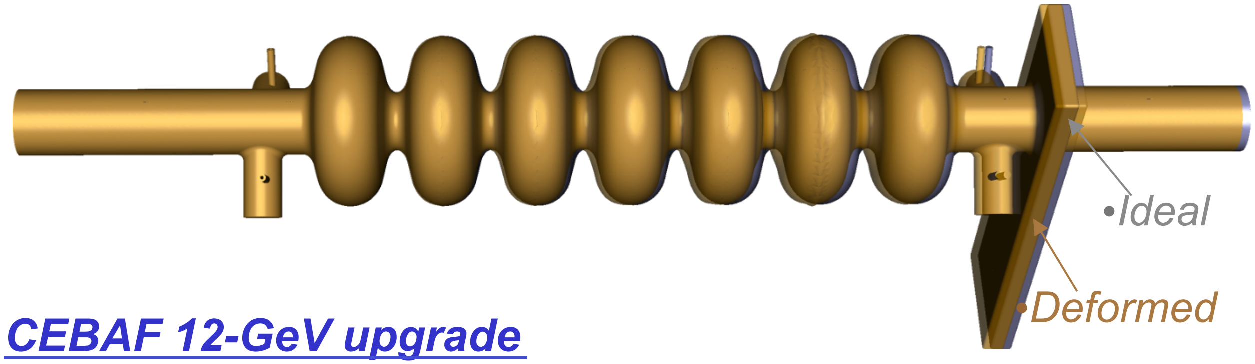
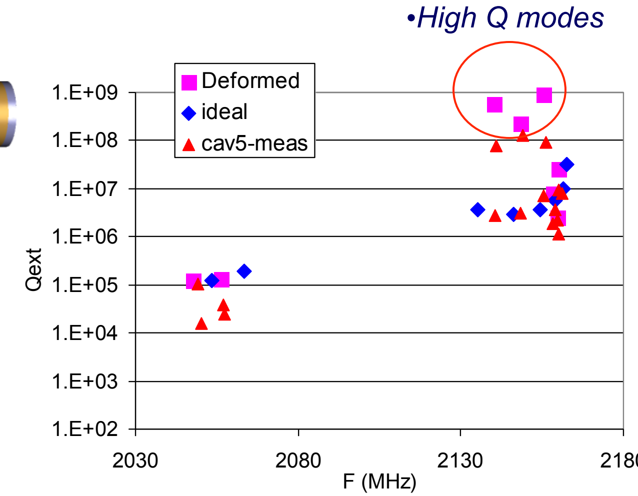
Beam Breakup in RF cavity

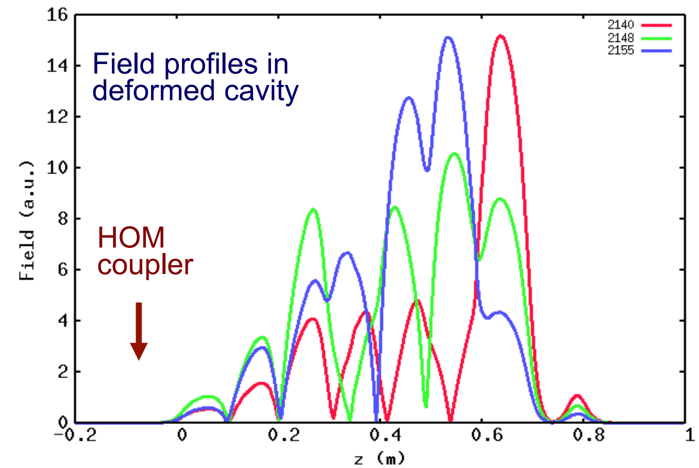




CEBAF 12-GeV upgrade

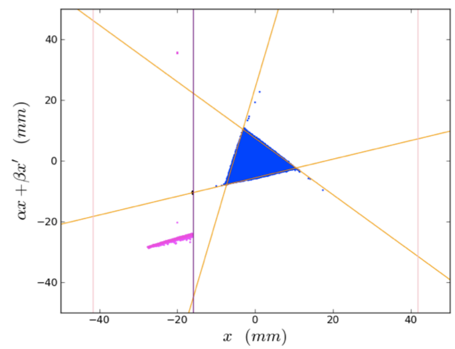
- Beam breakup (BBU) observed at beam currents well below design threshold
- Used measured RF parameters as input
- Solutions to the inverse problem identified the main cause of the BBU instability: **cavity is 8 mm short – *confirmed later from measurements***
- Combination of **experimental data and ComPASS tools** enabled solution of a real accelerator problem

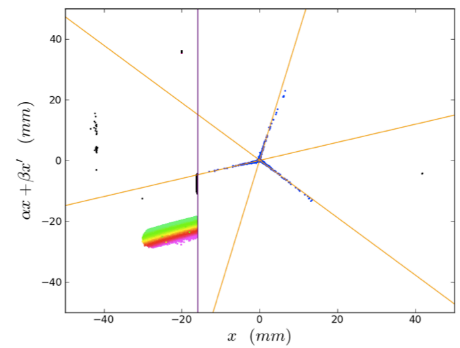
ACE3P

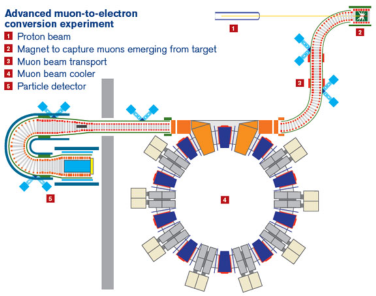


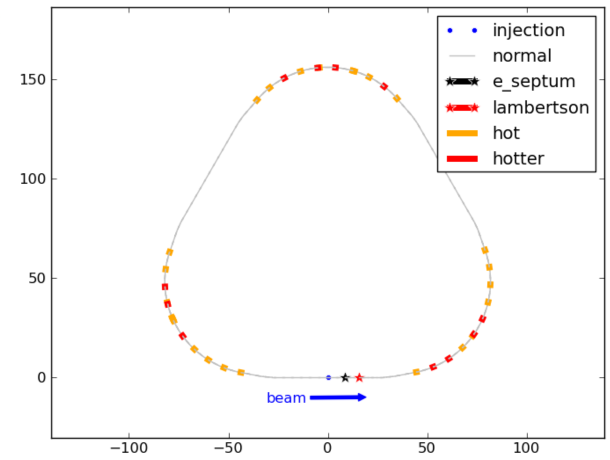
Intensity Frontier: Mu2e extraction design

- Synergia full extraction simulation for the Muon to Electron (Mu2e) Fermilab proposed experiment
  - 26k turns, 240 3D solves/turn, 1M macroparticles; include apertures and non-linear fields
  - Quantitative loss predictions
- Results contributed to CD1 approval for the experiment
- Only possible because of performance improvement obtained under SciDAC2!
- Activity is continuing but supported by the experiment
  - SciDAC supported development moves to “mainstream” production!









Summary

- Particle Accelerators are the most important instruments of discovery in HEP
  - in addition, they have many quality-of-life-enhancing applied science and industrial applications outside HEP
- Numerical modeling and simulation are essential for the development of new concepts and technologies and design and operation optimization
  - because of the complexity and many scales involved HPC is required for model fidelity
- ComPASS under SciDAC3 will develop and deploy state-of-the-art HPC accelerator modeling tools
  - major collaboration (and opportunity for) with SciDAC institutes
  - already mature tools and presence both in SciDAC and the community due to successful SciDAC2 ComPASS campaign